

INVESTIGATION OF PHASE TRANSITIONS IN SUBMONOLAYER HEXANE PHYSISORBED ONTO THE BASAL PLANE OF GRAPHITE

Cary L. Pint^{1,3}, Michael W. Roth¹, and Carlos Wexler²

¹ Department of Physics, University of Northern Iowa, Cedar Falls, IA 50614

² Department of Physics and Astronomy, University of Missouri-Columbia, MO 65211

³ Author to whom correspondence should be made. Email: cp489877@uni.edu

Abstract

We present the results of Molecular Dynamics (MD) simulations of hexane physisorbed onto the basal plane of graphite at different submonolayer coverages. We use a method of uniformly expanding the computational cell to simulate the submonolayer regime of $1 > \rho > 0.87$. Similar to full monolayer coverage, the system arranges in a solid herringbone phase at low temperatures. We find that the temperature of the solid-to-nematic and the nematic-to-melting phase transitions are both affected by the system's average density – a phenomenon also seen in experimental work. We examine and discuss the energetics, coordinate distributions, and order parameters for four submonolayer densities to give insight into the nature of the two transitions exhibited, and to further understand how the system evolves into the even more fascinating structures which have been observed experimentally at lower densities.